

Development of the GPS-met (IPW) Forward Model and Adjoint

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Backgound



- About 1.5 years ago I was asked by our group to devise an adjoint for GPS zenith IPW for the new variational system we were undertaking, since I had been assimilating GPW zenith IPW in the older LAPS system.
- Without any idea of what an adjoint was, I agreed to code this up.
- I learned quite a bit through this exercise and thought it worthwhile to share.

Outline



- Review forward model (FM) development and multi-grid implications for a FM
- Adjoint development process a methodology for other data sources
- Testing the adjoint
 - Discrete testing
 - Testing with the solver (solution engine inside vLAPS) with this FM and adjoint
- Summary

Outline



- Development here is for vLAPS.
 - However, it is important to note that the basic adjoint and forward model ideas are valid for other variational solution methods.
 - Adjoints are explicitly tied to the forward model.
- Adjoints are frequently mentioned in our work, it is hoped this presentation will help all to understand what adjoints are, how they can be developed, and how they are applied.

Outline



- This is a "how to" talk.
- WARNING: Technical methods using Calculus will be employed, efforts were taken to make this presentation easy to understand.
- Take this simple forward model case as an example for more complex systems. One can see how attention to detail is vital to success.

Math



The Calculus refresher:

$$\frac{\partial}{\partial q_i}(q_i) = 1 \qquad \frac{\partial}{\partial q_i}(q_{i\neq i}) = 0$$

$$\frac{d}{dx}\left(\frac{1}{2}u^2\right) = u\frac{d}{dx}f(x); \quad \frac{\partial}{\partial q_i}\left(\frac{1}{2}u^2\right) = u\frac{\partial}{\partial q_i}f(q)$$

Terms

- Forward model (FM) as used here, it
 integrates the specific humidity control variable resulting in a analysis version of the measured quantity of total precipitable water (TPW) directly comparable with GPS-met data, a zenith total precipitable water observation. (AKA observation operator)
- *J*, the penalty term, is computed from the FM value and the observation.
- Minimization gets into the subject of 3 and 4DVAR which is not discussed directly in this presentation.

Terms

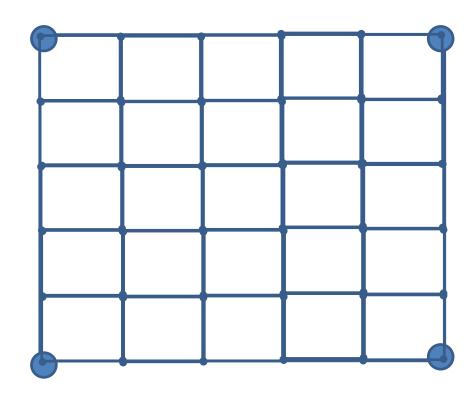


- Adjoint gradient J with regard to a control variable at i,j,k. Computed for gridpoints surrounding the observation location. Understand that an adjoint aids in solving for the minimum in the variational solver.
- You can have a bad adjoint and still solve, but it will not be as efficient as the correct adjoint. There are methods that solve without an adjoint, and though they are slow, they have their place (i.e., non-linear forward models)

Desired final grid

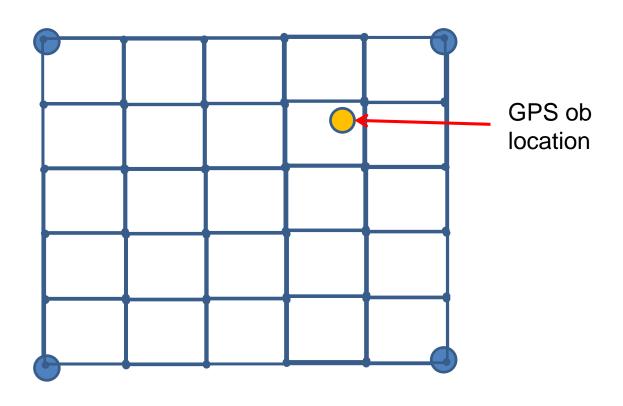


Top view, or one "k" level.



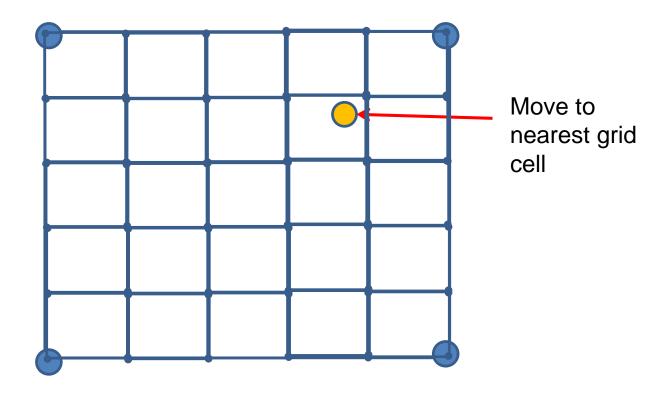
Observation within the grid





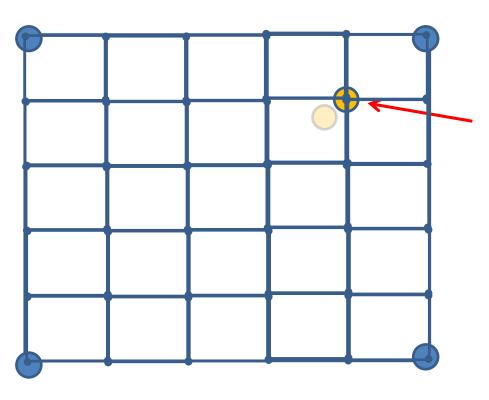
Old approximation not used in vLAPS





Old approximation not used in vLAPS





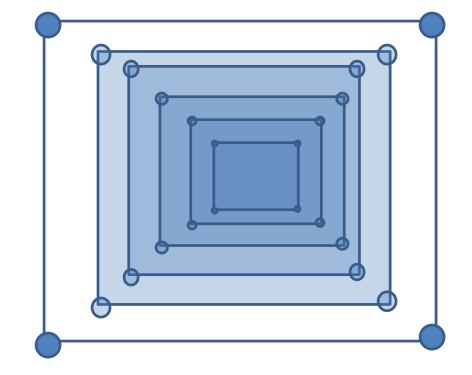
Move to nearest grid location and solve "approximating" this as the data location.

Multi-grid method



In vLAPS, work is done in "multigrids" one grid cell at a time, but the cell size shrinks as higher resolutions are solved.

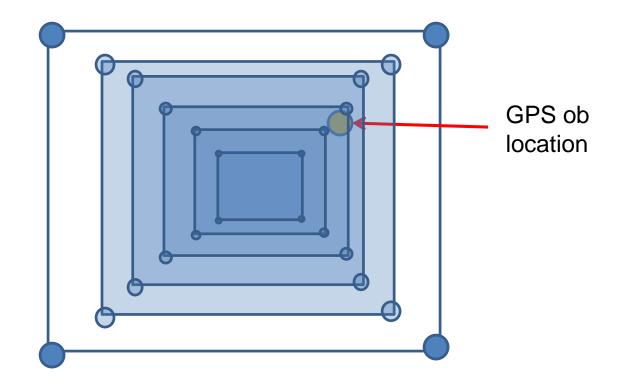
As subgrids are refined, cells approach the fine-scale grid dimensions.



Grid – ob location issue



As sub grids are invoked in solution, the observation location changes relative to the different subgrids.

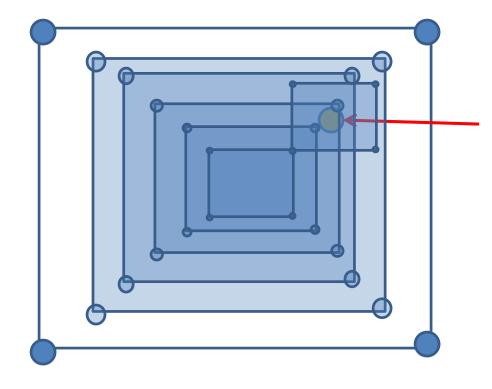


Reconciling the ob with regard to the grid scale



In fact, at the finer scales, the observation may change to a "different" grid cell. The observation in one subgrid could be very near a cell corner only to occupy the central part of a higher resolution subgrid.

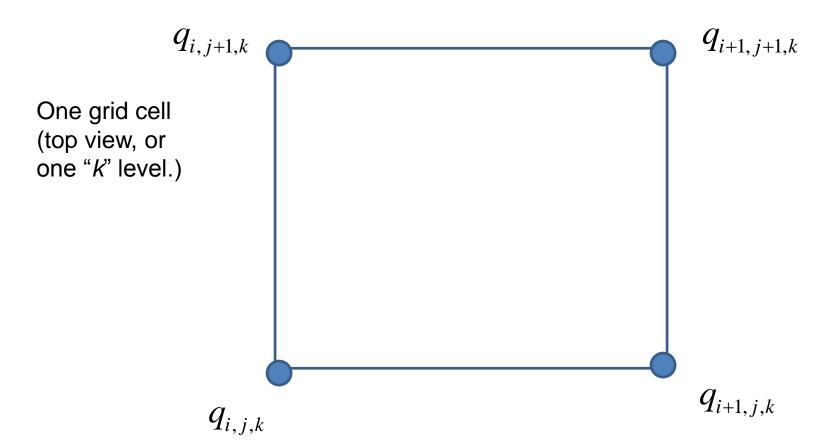
Regardless, corner indices change with each grid.



In the finest grid resolution, the ob might wind up in a whole different cell from the start. But each subgrid always employs different *i,j* corner points.

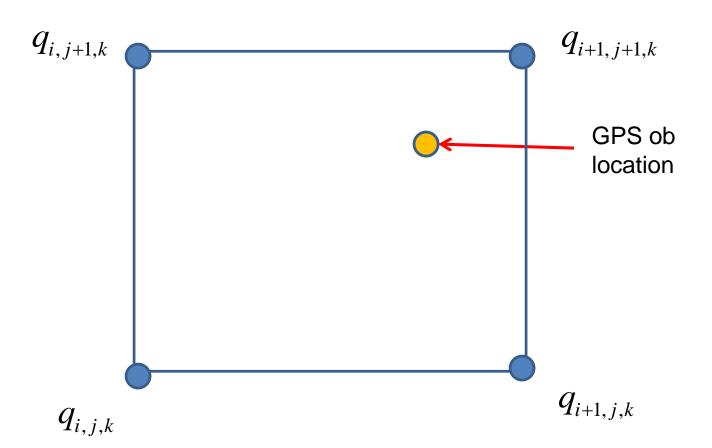
Unit grid (scale independent)





Observation location is arbitrary



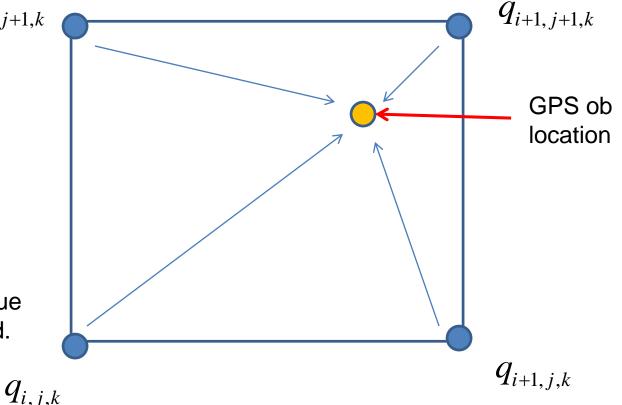


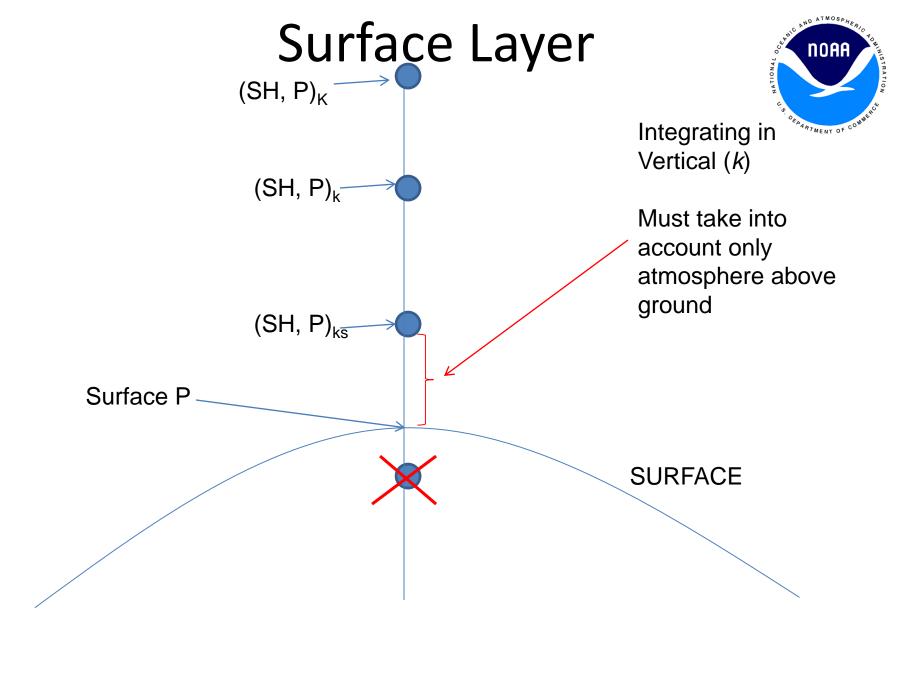
Unit cell solution - Independent of single/multi grid



 $q_{i,j+1,k}$ How to handle subgrids?

Bilinear interpolation of the control variable data to GPS observation location – unique to each subgrid.









 $q_{i+1,j,k}$

 $q_{i,j+1,k}$ Bilinear interpolation of control variable data to the GPS observation location is done uniquely for all subgrids. $q_{i,j,k}$ EXACT GPS ob location $\sum_{k=1}^{K} I_k \text{ Is the FM !}$

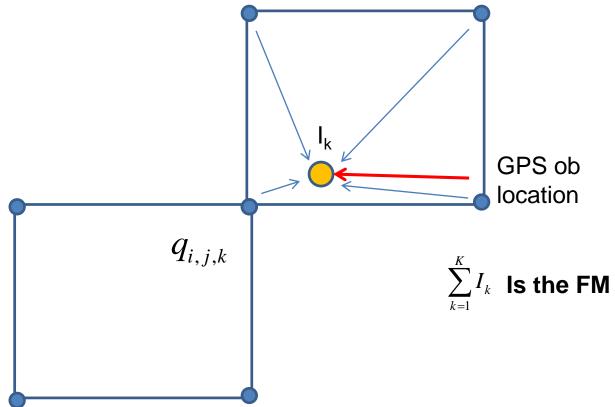
 I_k = water at level k computed from the control variable "q"

$$J = 1/2(\sum_{k=1}^{K} I_k - GPS observation)^2$$
 where J is the minimized functional

Concept of a FM



Bilinear interpolation of control variable data to the GPS observation location is done uniquely for all subgrids.

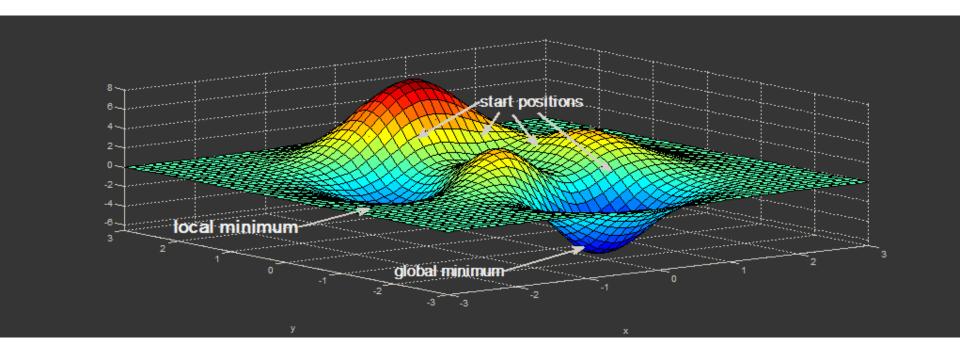


 I_k = water at level k computed from the control variable "q"

$$J = 1/2(\sum_{k=1}^{K} I_k - \text{GPS observation})^2$$
 where J is the minimized functional

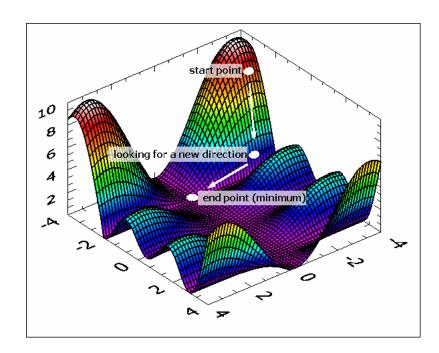
Objective is to minimize J - the core of 3|4DVAR





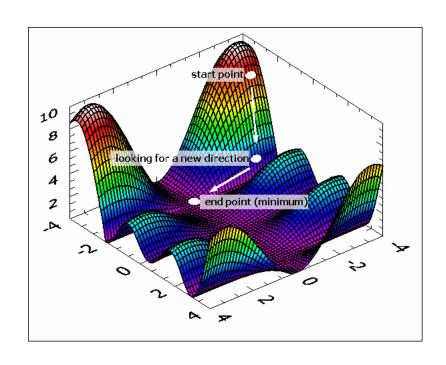
Most solution methods utilize information about the slope in the region of the solution, to aid in iteration increments to find the minimum as efficiently as possible. This is the role of the adjoint.

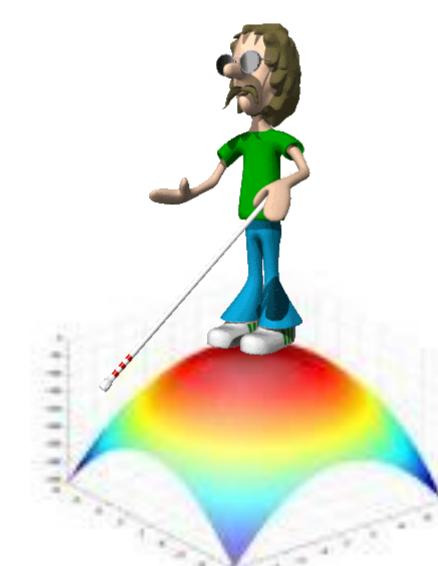




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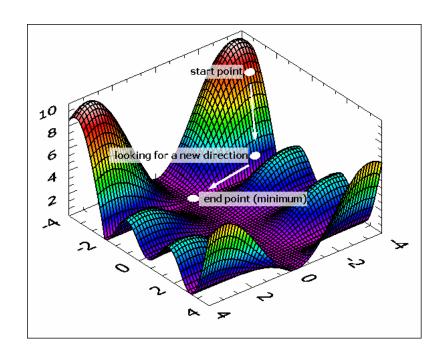


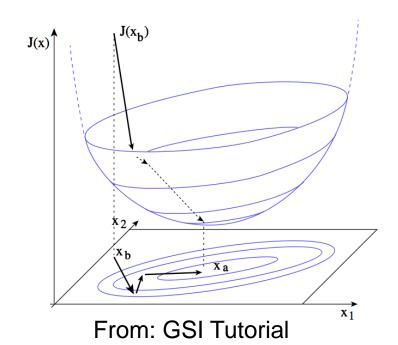




Most solution methods utilize information about the slope in the region of the solution, to aid in iteration increments to find the minimum as efficiently as possible. This is the role of the adjoint.







Define the forward model (FM)



$$I = \int_{p_{-}sfc}^{p_{-}top} \frac{q}{g} dp$$

This integral can be formulated to units of $I = \int_{p_-sfc}^{p_-top} \frac{q}{g} dp$ centimeters to match GPS. But we move the "g" term to modify TPW to be in the same units as vLAPS q.

vLAPS
$$q$$
.
$$I = \sum_{k=ks}^{K} \overline{q}_k \ \Delta p_k + "moisture \ above the \ surface \ to \ ks"$$

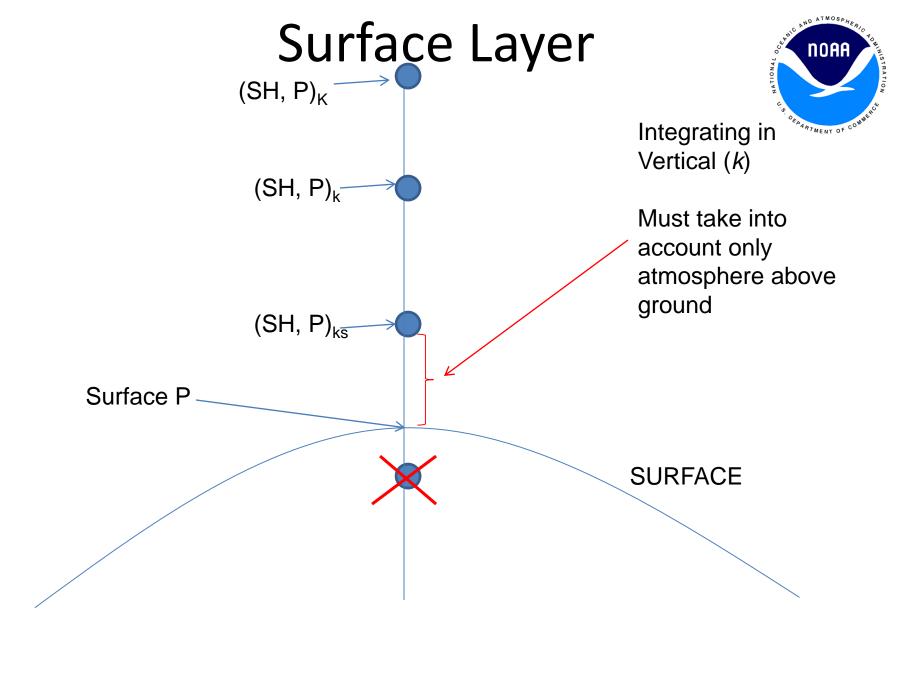
$$I = \sum_{k=ks}^{K-1} \frac{(q_k + q_{k+1})}{2} \Delta p_k + q_{ks} (p_{sfc} - p_{ks})$$

$$I = \sum_{k=ks}^{K-1} \frac{(q_k + q_{k+1})}{2} (p_k - p_{k+1}) + q_{ks} (p_{sfc} - p_{ks})$$

Define the penalty term or functional to minimize (J)

$$J = \frac{1}{2}(I - \text{GPS observation}^*)^2$$

^{*} GPS here has been modified as TPW*g*100. to match g/kg & hPa units.



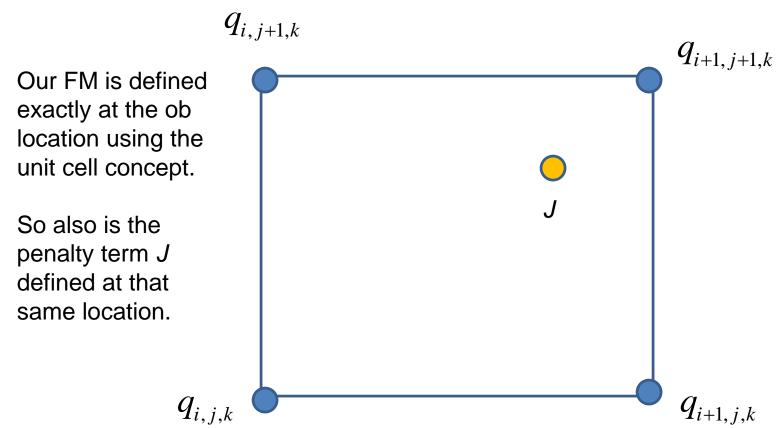
This is **NOT** at all similar to the "old LAPS"



- The forward model in the K dimension is similar to old LAPS. (perhaps the only thing)
- Cannot use nearest gridpoint assignment.
- Bilinear interpolation (nearest neighbor) is used instead.
- vLAPS uses an adjoint for accelerating solution convergence, old LAPS didn't do this - next we look at the adjoint

Concept of the Adjoint





I = integrated water through the vertical at all k level computed from the control variable "q"

 $J = 1/2(I - GPS observation)^2$

Just what is an adjoint?



- The GPS adjoint is the partial derivative of J (at the GPS location) with respect to a control variable. It is must be spread to the 4 gridpoints surrounding the J location. The assignment of the partial derivative at the 4 points through bilinear interpolation using the same weights used for the FM.
- The adjoint is used in the solver to modify the control variables on the grid, thus changing the FM value at the ob location.
- If the adjoint value is **zero**, **there will be no change to a control variable**. Typically it is zero except around the cell containing the ob. Note the adjoint becomes zero when the FM = observation, e.g., solution!
- The derived adjoint can be **incorrect** and the solver **may** still converge. Usually this is the case if it is wrong in magnitude. The solver may not converge at all if the adjoint is wrong in sign (+/-).

Computation of the partial derivative of J WRT q at level k



$$J = \frac{1}{2}(I - \text{GPS observation})^2$$

$$\frac{\partial J}{\partial q_k} = (I - \text{GPS observation}) \frac{\partial}{\partial q_k} I$$

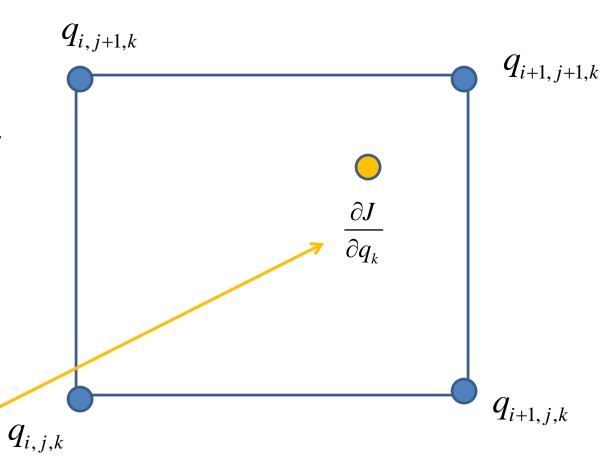
$$\frac{\partial J}{\partial q_k} = (I - \text{GPS observation}) \frac{\partial}{\partial q_k} \left\{ \sum_{k=k_s}^{K-1} 0.5 \left(q_k + q_{k+1} \right) \left(p_k - p_{k+1} \right) + \text{"bottom of column"} \right\}$$

$$\frac{\partial J}{\partial q_k} = (I - \text{GPS observation}) \frac{\partial}{\partial q_k} \left\{ \sum_{k=k_s}^{K-1} 0.5 \left(q_k + q_{k+1} \right) \left(p_k - p_{k+1} \right) + q_{ks} \left(p_{sfc} - p_{ks} \right) \right\}$$





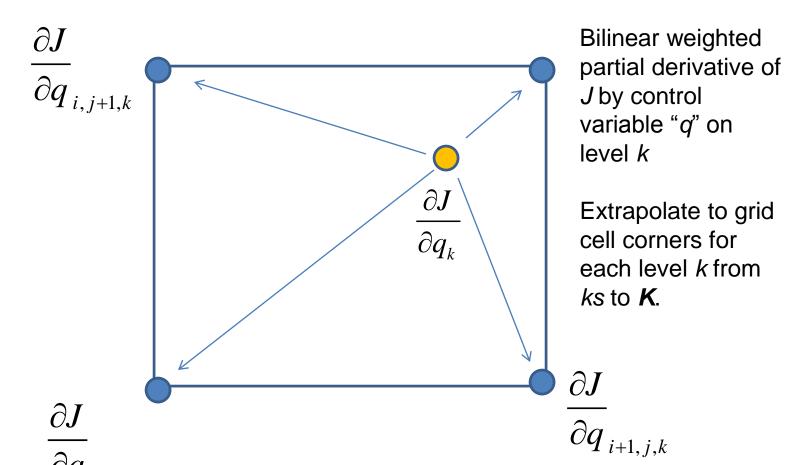
Take the partial derivative of *J* at level *k* with respect to the control variable *q*.

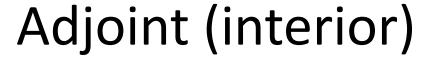


$$\frac{\partial J}{\partial q_k} = (I - \text{GPS observation}) \frac{\partial}{\partial q_k} \left\{ \sum_{k=k_s}^{K-1} 0.5 \left(q_k + q_{k+1} \right) \left(p_k - p_{k+1} \right) + q_{ks} \left(p_{sfc} - p_{ks} \right) \right\}$$

Concept of Adjoint





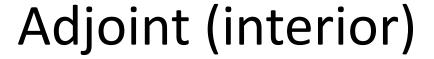




$$\frac{\partial J}{\partial q_k} = (I - \text{GPS observation}) \frac{\partial}{\partial q_k} \left\{ \sum_{k=k_s}^{K-1} 0.5 \left(q_k + q_{k+1} \right) \left(p_k - p_{k+1} \right) + q_{ks} \left(p_{sfc} - p_{ks} \right) \right\}$$

Note that due to the nature of indices, level "k" will appear more than once when the above is expanded, here look at terms 1-5 and focus on "3".

$$\frac{\partial J}{\partial q_k} = (I - \text{GPS observation}) [0.5(q_1 + q_2) (p_1 - p_2) + 0.5(q_2 + q_3) (p_2 - p_3) + 0.5(q_3 + q_4) (p_3 - p_4) + 0.5(q_4 + q_5) (p_4 - p_5) \cdots + 0.5(q_k + q_{k+1}) (p_k - p_{k+1}) + q_{ks} (p_{sfc} - p_{ks})]$$





$$\frac{\partial J}{\partial q_k} = (I - \text{GPS observation}) \frac{\partial}{\partial q_k} \left\{ \sum_{k=k_s}^{K-1} 0.5 \left(q_k + q_{k+1} \right) \left(p_k - p_{k+1} \right) + q_{ks} \left(p_{sfc} - p_{ks} \right) \right\}$$

Note that due to the nature of indices, level "k" will appear more than once when the above is expanded, here look at terms 1-5 and focus on "3".

$$\frac{\partial J}{\partial q_{3}} = (I - \text{GPS observation}) [0.5(q_{1} + q_{2}) (p_{1} - p_{2}) + 0.5(q_{2} + 1) (p_{2} - p_{3}) + 0.5(1 + q_{4}) (p_{3} - p_{4}) + 0.5(q_{4} + q_{5}) (p_{4} - p_{5})$$
...
$$+ 0.5(q_{k} + q_{k+1}) (p_{k} - p_{k+1}) + q_{ks}(p_{sfc} - p_{ks})]$$

Adjoint (interior)



$$\frac{\partial J}{\partial q_k} = (I - \text{GPS observation}) \frac{\partial}{\partial q_k} \left\{ \sum_{k=k_s}^{K-1} 0.5 \left(q_k + q_{k+1} \right) \left(p_k - p_{k+1} \right) + q_{ks} \left(p_{sfc} - p_{ks} \right) \right\}$$

Note that due to the nature of indices, level "k" will appear more than once when the above is expanded, here look at terms 1-5 and focus on "3".

$$\frac{\partial J}{\partial q_3} = (I - \text{GPS observation}) [$$

$$+ 0.5 (p_2 - p_3)$$

$$+ 0.5 (p_3 - p_4)]$$

$$\frac{\partial J}{\partial q_3} = (I - \text{GPS observation}) [0.5 (p_2 - p_4)]$$

Adjoint (interior)



$$\frac{\partial J}{\partial q_k} = (I - \text{GPS observation}) \frac{\partial}{\partial q_k} \left\{ \sum_{k=k_s}^{K-1} 0.5 \left(q_k + q_{k+1} \right) \left(p_k - p_{k+1} \right) + q_{ks} \left(p_{sfc} - p_{ks} \right) \right\}$$

Note that due to the nature of indices, level "k" will appear more than once when the above is expanded, here look at terms 1-5 and focus on "3".

$$\frac{\partial J}{\partial q_3} = (I - \text{GPS observation}) [$$

$$+ 0.5 (p_2 - p_3)$$

$$+ 0.5 (p_3 - p_4)]$$

$$\frac{\partial J}{\partial q_3} = (I - \text{GPS observation}) [0.5 (p_2 - p_4)]$$

$$\frac{\partial J}{\partial q_k} = (I - \text{GPS observation}) [0.5 (p_{k-1} - p_{k+1})]$$

Adjoint (interior)



$$\frac{\partial J}{\partial q_k} = (I - \text{GPS observation}) [0.5 (p_{k-1} - p_{k+1})]$$

Is valid for interior of the column only. k .ne. **K**, and k .ne. ks The top and bottom cells are special cases.

• It is very important to note that the (*I*-GPS ob) difference determines the SIGN of the gradient. Also the sign can be incorrect if you have made an error in the *i*, *j*, or *k* indices.

Concept of Adjoint (top)



$$\frac{\partial J}{\partial q_k} = (I - \text{GPS observation}) \frac{\partial}{\partial q_k} \left\{ \sum_{k=k_s}^{K-1} 0.5 \left(q_k + q_{k+1} \right) \left(p_k - p_{k+1} \right) + q_{ks} \left(p_{sfc} - p_{ks} \right) \right\}$$

Now look at K, the top special case. Here call it "5" where 5=K and 4 = K-1 and we assume there is no "6" because "5" is at the top.

$$\frac{\partial J}{\partial q_5} = (I - \text{GPS observation}) [0.5(q_4 + 1) (p_4 - p_5)]$$

Concept of Adjoint (top)



$$\frac{\partial J}{\partial q_k} = (I - \text{GPS observation}) \frac{\partial}{\partial q_k} \left\{ \sum_{k=k_s}^{K-1} 0.5 \left(q_k + q_{k+1} \right) \left(p_k - p_{k+1} \right) + q_{ks} \left(p_{sfc} - p_{ks} \right) \right\}$$

Now look at K, the top special case. Here call it "5" where 5=K and 4 = K-1 and we assume there is no "6" because "5" is at the top.

$$\frac{\partial J}{\partial q_5} = (I - \text{GPS observation}) [0.5(q_4' + 1) (p_4 - p_5)]$$

$$\frac{\partial J}{\partial q_K} = (I - \text{GPS observation}) [0.5 (p_{K-1} - p_K)]$$

Concept of Adjoint (bottom)



$$\frac{\partial J}{\partial q_k} = (I - \text{GPS observation}) \frac{\partial}{\partial q_k} \left\{ \sum_{k=k_s}^{K-1} 0.5 \left(q_k + q_{k+1} \right) \left(p_k - p_{k+1} \right) + q_{ks} \left(p_{sfc} - p_{ks} \right) \right\}$$

Now look at ks (and sfc), the bottom special case. Index ks.

$$\frac{\partial J}{\partial q_{ks}} = (I - \text{GPS observation}) \frac{\partial}{\partial q_{ks}} \left\{ \sum_{k=k_s}^{K-1} 0.5 \left(q_k + q_{k+1} \right) \left(p_k - p_{k+1} \right) + q_{ks} \left(p_{sfc} - p_{ks} \right) \right\}$$

$$\frac{\partial J}{\partial q_{ks}} = (I - \text{GPS observation}) \left[0.5(1 + q_{ks+1}) \left(p_{ks} - p_{ks+1} \right) + 1(p_{sfc} - p_{ks}) \right]$$

$$\frac{\partial J}{\partial q_s} = (I - \text{GPS observation}) \left[0.5 \left(p_{ks} - p_{ks+1} \right) + \left(p_{sfc} - p_{ks} \right) \right]$$

Concept of Adjoint (bottom)



$$\frac{\partial J}{\partial q_k} = (I - \text{GPS observation}) \frac{\partial}{\partial q_k} \left\{ \sum_{k=k_s}^{K-1} 0.5 \left(q_k + q_{k+1} \right) \left(p_k - p_{k+1} \right) + q_{ks} \left(p_{sfc} - p_{ks} \right) \right\}$$

Now look at *ks* (and sfc), the bottom special case. Index *ks*.

$$\frac{\partial J}{\partial q_{ks}} = (I - \text{GPS observation}) \frac{\partial}{\partial q_{ks}} \left\{ \sum_{k=k_s}^{K-1} 0.5 \left(q_k + q_{k+1} \right) \left(p_k - p_{k+1} \right) + q_{ks} \left(p_{sfc} - p_{ks} \right) \right\}$$

$$\frac{\partial J}{\partial q_{ks}} = (I - \text{GPS observation}) \left[0.5(1 + q_{ks+1}) \left(p_{ks} - p_{ks+1} \right) + 1(p_{sfc} - p_{ks}) \right]$$

Don't make this mistake

$$\frac{\partial J}{\partial a_s} = (I - \text{GPS observation}) \left[0.5 \left(p_{ks} - p_{ks+1} \right) + \left(p_{sfc} - p_{ks} \right) \right]$$

Full Numerical Adjoint



$$\frac{\partial J}{\partial q_k} = (I - \text{GPS observation}) \frac{\partial}{\partial q_k} \left\{ \sum_{k=k_s}^{K-1} 0.5 \left(q_k + q_{k+1} \right) \left(p_k - p_{k+1} \right) + q_{ks} \left(p_{sfc} - p_{ks} \right) \right\}$$

The full adjoint has 3 parts to it. Top, middle, and near-surface.

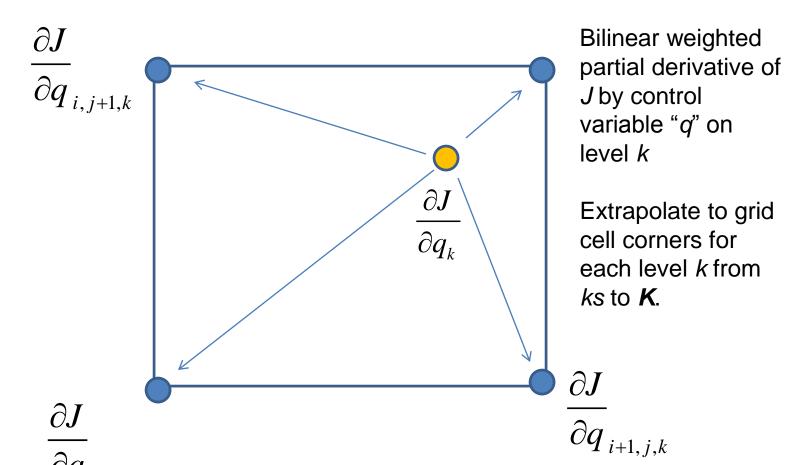
$$\frac{\partial J}{\partial q_K} = (I - \text{GPS observation}) [0.5 (p_{K-1} - p_K)]$$

$$\frac{\partial J}{\partial q_k} = (I - \text{GPS observation}) [0.5 \ (p_{k-1} - p_{k+1})]$$

$$\frac{\partial J}{\partial q_{ks}} = (I - \text{GPS observation}) \left[0.5 \left(p_{ks} - p_{ks+1} \right) + \left(p_{sfc} - p_{ks} \right) \right]$$

Concept of Adjoint





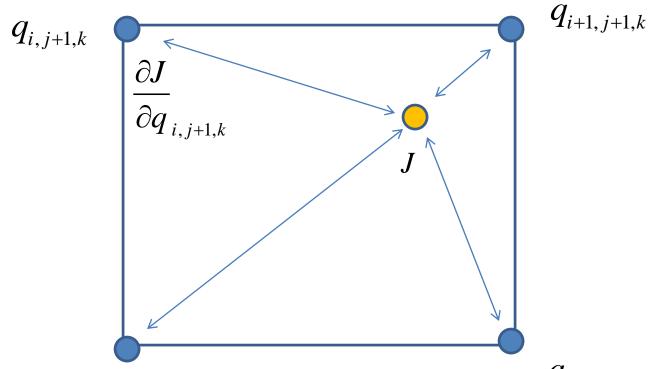
Adjoint Testing



- Example, test $\frac{\partial J}{\partial q_{i,j,k}}$ for each place in the grid where it exists.
- Use perturbation and the forward model at ONE GRIDPOINT to approximate associated partial derivative of J by changing $q_{i,j,k}$ by $q_{i,j,k} + \Delta q_{i,j,k}$.
- Perform for all control-variable gridpoints and see if adjoint partials, match thusly computed partials.

Adjoint test



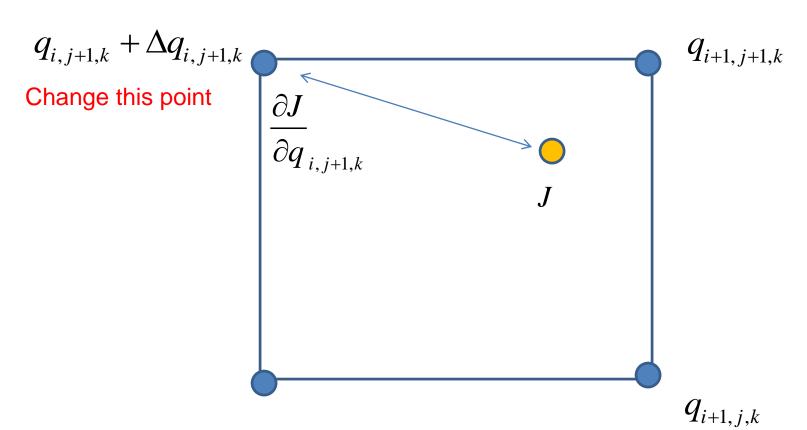


 $q_{i,j,k}$

 $q_{i+1,j,k}$

Adjoint test (cont.)

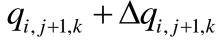




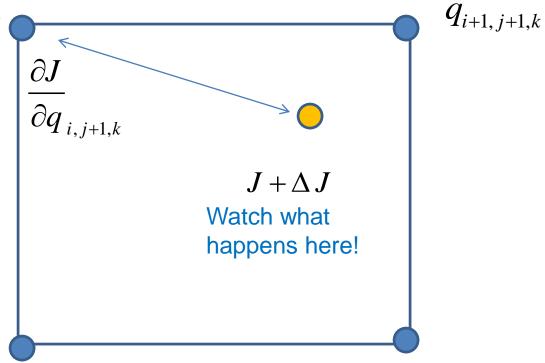
 $q_{i,j,k}$

Adjoint test (cont.)





Change this point



$$q_{i,j,k}$$

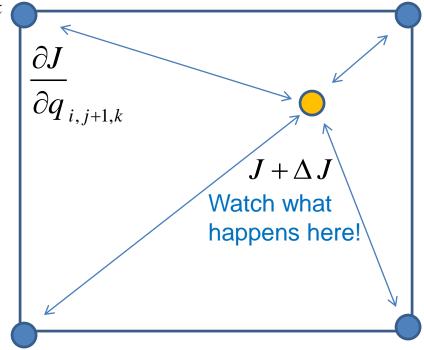
$$q_{i+1,j,k}$$

Adjoint test (cont.)



$$q_{i,j+1,k} + \Delta q_{i,j+1,k}$$

Change this point



Compare:

$$rac{\Delta J}{\Delta q}_{i,j+1,k}$$
 FM effect

With

$$\frac{\partial J}{\partial q}_{i,j+1,k}$$
 adjoint

$$q_{i+1,j,k}$$



• The trick is usually to increase $\Delta q_{i,j,k}$ not decrease it!

Solver Test

- Place the Forward model AND adjoint into the solver routine by themselves and see if convergence occurs.
- This is external to vLAPS but uses the same solver (important, you study this without other data)
- Important, since if you put it into vLAPS
 without this test being successful, you don't
 know what might be going on.

Solver Test Output

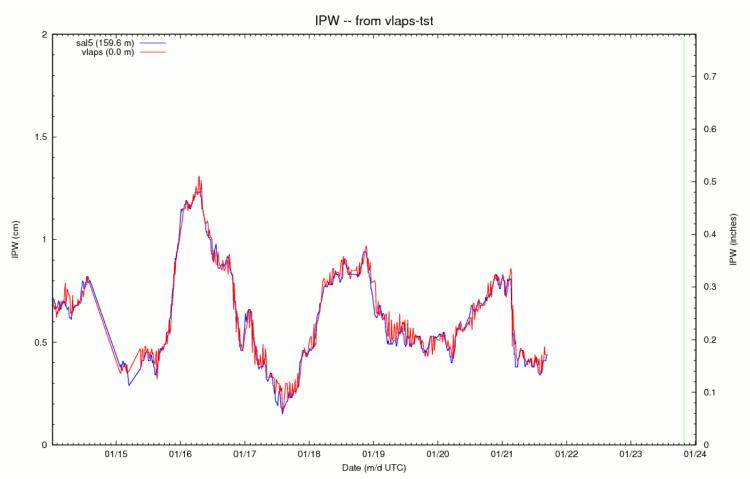


```
RUNNING THE L-BFGS-B CODE
Machine precision = 2.220D-16
N = 6162373 M = 14
At X0 0 variables are exactly at the bounds
j gps changing 10.82477
At iterate 0 f= 1.08248D+01 |proj g|= 1.20899D-01
j gps changing 10.72041
At iterate 1 f = 1.07204D + 01 |proj g|= 1.20337D-01
j gps changing 0.2229756
At iterate 2 f= 2.22976D-01 |proj g|= 3.32823D-02
j gps changing 2.651105
j gps changing 0.1068712
At iterate 3 f = 1.06871D - 01 |proj g| = 1.02766D - 02
j gps changing 5.9161554E-03
At iterate 4 f= 5.91616D-03 |proj g|= 3.64435D-03
j qps changing 1.8386532E-02
j gps changing 4.5083204E-04
At iterate 5 f= 4.50832D-04 |proj g|= 7.51569D-04
j gps changing 9.4540301E-05
At iterate 6 f= 9.45403D-05 |proj g|= 2.33093D-04
j gps changing 2.1491633E-05
At iterate 7 f= 2.14916D-05 |proj g|= 1.60543D-04
j gps changing 8.4271760E-06
At iterate 8 f= 8.42718D-06 |proj g|= 9.71679D-05
j gps changing 2.0542170E-06
At iterate 9 f= 2.05422D-06 |proj q|= 3.19417D-05
j gps changing 2.0960721E-07
At iterate 10 f= 2.09607D-07 |proj g| = 8.97315D-06
```

```
Tit = total number of iterations
Tnf = total number of function evaluations
Thint = total number of segments explored during
Cauchy searches
Skip = number of BFGS updates skipped
Nact = number of active bounds at final generalized
Cauchy point
Projg = norm of the final projected gradient
F = final function value
N Tit Tnf Tnint Skip Nact Projg F
***** 10 13 53 0 0 8.973D-06 2.096D-07
F = 2.0960720803486765E-007
CONVERGENCE: NORM OF PROJECTED GRADIENT <= PGTOL
Cauchy time 2.640E+00 seconds.
Subspace minimization time 1.929E+01 seconds.
Line search time 1.365E+01 seconds.
```

Analysis Performance

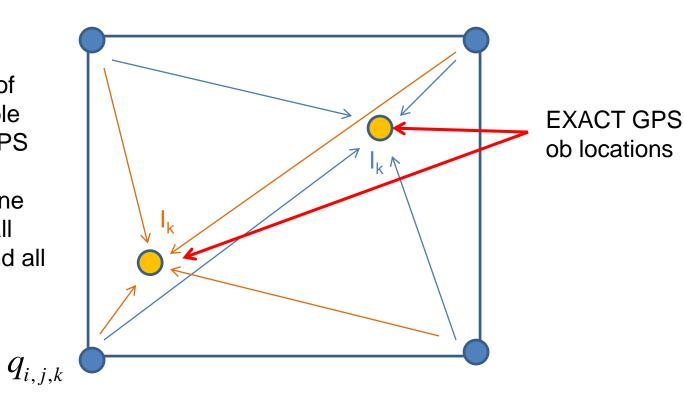




Concept of a FM Multiple obs



Bilinear interpolation of control variable data to the GPS observation location is done uniquely for all subgrids – and all obs within a subgrid.



Unique J for each ob location

Multi-ob adjoints



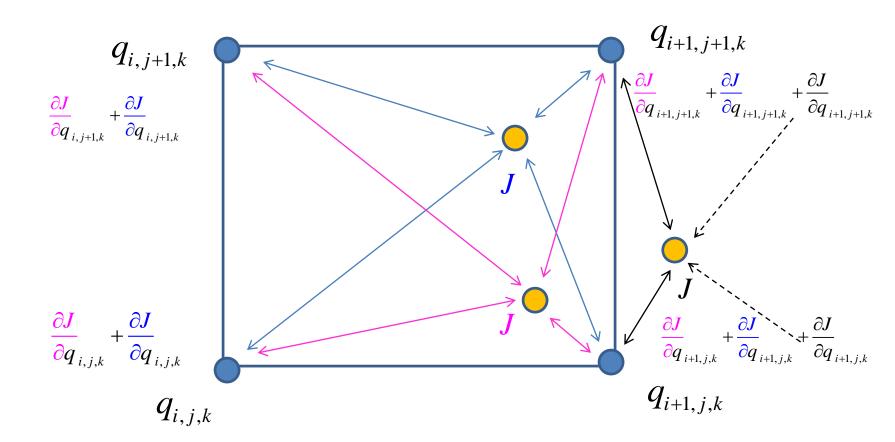
 $q_{i+1,j,k}$

$$\frac{\partial J}{\partial q_{i,j+1,k}} + \frac{\partial J}{\partial q_{i,j+1,k}} + \frac{\partial J}{\partial q_{i+1,j+1,k}} + \frac{\partial J}{\partial q_{i+1,j+1,k}} + \frac{\partial J}{\partial q_{i+1,j+1,k}} + \frac{\partial J}{\partial q_{i+1,j,k}} + \frac{\partial J}{\partial q_{i+1,j,k}} + \frac{\partial J}{\partial q_{i+1,j,k}}$$

 $q_{i,j,k}$

Multi-ob adjoints





Summary



- The forward model describes the observation using surrounding control variables.
- The J functional compares the FM result to an observation and is used to identify minimization (solved fit).
- The adjoint is derived from the FM. Imperfect adjoints can still work, but efficiency will be lost. There is only ONE true adjoint for a FM.
- The adjoint accelerates the solution operation.

Summary (2)



- Watch for index errors in coding. They are hard to spot and will really cause problems.
- Even though a poor adjoint can allow the system to solve, a sign error can cause the system to always overshoot in the wrong direction winding up with an inability to converge, or very very slow convergence.
- The multi-grid approach allows for memory of the control variable fields as one goes to more and more dense grids. For this reason only one "cell" around the measurement needs an adjoint computation.

Summary (3)



- Multiple observations within a cell (especially likely at coarse initial grid sizes), will result in more than one partial derivative at a cell's grid points. This is handled by summing the derivatives.
- Also, observations in adjacent cells will generate partial derivatives at the 2 shared grid points. Again, this situation is handled by summing the derivatives there together to get the adjoint.

Summary (4)



- For testing, remember to test the numerical approximation for the adjoint with the Calculus version first.
- When testing with the solver, test with numerical solver alone. This will not mix its performance with other solved variables.
- The last step is to incorporate the adjoint with others in the multivariate solver to combine the solution with other observations.

Summary (5)



- Final word of caution.
- Just because you have added a new observation to your analysis, you are not guaranteed to see associated model performance improve. Obviously this is the desired result, but your model may do things you "don't know about." Your new observations might "throw off" bias corrections you don't know about in the model. In many ways, the model is a black box to your efforts. If you are lucky, you will have a better forecast.